A mixed mean-field/BCS phase
with an energy gap at high T_c

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Abstract

We construct a pair potential which in a scaling limit leads to a Hamiltonian that generates co-existing mean-field and superconducting phases. Depending on the relative values of the coupling constants, the superconducting phase may exist at arbitrarily high temperatures.

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Introduction

In quantum mechanics a mean field theory means that the particle density $\rho(x) = \psi^*(x)\psi(x)$ (in second quantization) tends to a c-number in a suitable scaling limit. Of course, $\rho(x)$ is only an operator valued distribution and the smeared densities $\rho_f = \int dx\, \rho(x)f(x)$ are (at best) unbounded operators, so norm convergence is not possible. The best one can hope for is strong resolvent convergence in a representation where the macroscopic density is built in. The BCS-theory of superconductivity is of a different type where pairs of creation operators with opposite momentum $\tilde\psi^*(k)\,\tilde\psi^*(-k)$ ($\tilde\psi$ the Fourier transform and with the same provisio) tend to c-numbers. This requires different types of correlations and one might think that the two possibilities are mutually exclusive. We shall show that this is not so by constructing a pair potential where both phenomena occure simultaneously. On purpose we shall use only one type of fermions as one might think that the spin-up electrons have one type of correlation and the spin-down the other. Also the state which carries both correlations is not an artificial construction but it is the KMS-state of the corresponding Bogoliubov Hamiltonian. Whether the phenomenon occurs or not depends on whether the emerging two coupled "gap equations" have a solution or not, which happens to be the case in certain regions of the parameter space (temperature, chemical potential, relative values of the two coupling constants). Moreover, in the new phases with $\lambda_B, \lambda_M < 0$ transition temperature T_c may become arbitrarily high. Our considerations hold for arbitrary space dimension.

1 Quadratic fluctuations in a KMS-state

The solvability of the BCS-model [1] rests upon the observation [2] that in an irreducible representation the space average of a quasi-local quantity is a c-number and is equal to its ground state expectation value. This allows one to replace the model Hamiltonian by an equivalent approximating one [3]. Remember that two Hamiltonians are considered to be equivalent when they lead to the same time evolution of the local observables [4].

The same property holds on also in a temperature state (the KMS-state) and under conditions to be specified later it makes the co-existence of other types of phases possible.

To make this apparent, consider the approximating (Bogoliubov) Hamiltonian

$$
\begin{aligned}
H'_B &= \int dp \left\{ \omega(p)a^*(p)a(p) + \frac{1}{2}\Delta_B(p)\left[a^*(p)a^*(-p) + a(-p)a(p)\right] \right\} \\
&= \int W(p)b^*(p)b(p)\,,
\end{aligned}
\tag{1.1}
$$

which has been diagonalized by means of a standard Bogoliubov transformation with real coefficients (the irrelevant infinite constant in H'_B has been omitted)

$$
b(p) = c(p)a(p) + s(p)a^*(-p)\,, \qquad a(p) = c(p)b(p) - s(p)b^*(-p)
$$

with

$$
c(p) = c(-p)\,, \qquad s(p) = -s(-p)\,, \qquad c^2(p) + s^2(p) = 1\,,
\tag{1.2}
$$

so that the following relations hold (keeping in mind that Δ, W, s, c will be β–dependent)

$$W(p) = \sqrt{\omega^2(p) + \Delta_B^2(p)} = W(-p)$$

$$c^2(p) - s^2(p) = \omega(p)/W(p), \qquad 2c(p)s(p) = \Delta_B(p)/W(p) \qquad (1.3)$$

Hamiltonian (1.1) generates a well defined time evolution and a KMS-state for the b-operators. For the original creation and annihilation operators a, a^* this gives the following evolution

$$a(p) \rightarrow a(p)\left(c^2(p)e^{-iW(p)t} + s^2(p)e^{iW(p)t}\right) - 2ia^*(-p)c(p)s(p)\sin W(p)t$$

and nonvanishing termal expectations

$$
\begin{aligned}
\langle a^*(p)a(p')\rangle &= \delta(p - p')\left\{\frac{c^2(p)}{1 + e^{\beta(W(p)-\mu)}} + \frac{s^2(p)}{1 + e^{-\beta(W(p)-\mu)}}\right\} \\
&:= \delta(p - p')\{p\} \qquad (1.4) \\
\langle a(p)a(-p')\rangle &= \delta(p - p')c(p)s(p)\tanh\frac{\beta(W(p) - \mu)}{2} := \delta(p - p')[p] \qquad (1.5)
\end{aligned}
$$

$$\{p\} = \{-p\}, \qquad [p] = -[-p]$$

c and s are multiplication operators and are never Hilbert–Schmidt. Thus different c and s lead to inequivalent representations and should be considered as different phases of the system.

The expectation value of a biquadratic (in creation and annihilation operators) quantity is expressed through (1.4,5)

$$
\langle a^*(q)a^*(q')a(p)a(p')\rangle = \delta(q + q')\delta(p + p')[q][p] - \\
-\delta(p - q)\delta(p' - q')\{p\}\{p'\} + \delta(p - q')\delta(p' - q)\{p\}\{p'\} \qquad (1.6)
$$

So far we have written everything in terms of the operator valued distributions $a(p)$. They can be easily converted into operators in the Hilbert space generated by the KMS-state by smearing with suitable test functions. Thus, by smearing with e.g.

$$e^{-\kappa(p+p')^2 - \kappa(q+q')^2}v(p)v(q), \qquad v \in L_2(\mathbf{R}^d) \qquad (1.7)$$

one observes that in the limit $\kappa \rightarrow \infty$ the first term in (1.6) remains finite

$$0 < \int dp\,dq\,v(p)v(q)[p][q] < \infty,$$

while the two others vanish

$$\lim_{\kappa \to \infty} \int dp\,dp'\,e^{-2\kappa(p+p')^2}v(p)v(p')\{p\}\{p'\} = \lim_{\kappa \to \infty} \kappa^{-3/2}\int dp\,v^2(p)\{p\}^2 = 0.$$

Since we are in the situation of *Lemma 1* in [5], we have thus proved the following statement

$$\text{s-}\lim_{\kappa\to\infty}\int dp\,dp'\,\mathcal{V}(q,q',p,p')e^{-\kappa(p+p')^2}a(p)a(p')=\int dp\,\mathcal{V}(q,q',p,-p)[p] \qquad (1.8)$$

for kernels $\mathcal{V}$ such that the integrals are finite.

With this observation in mind, a potential which acts for $\kappa\to\infty$ like (1.1) might be written as

$$V_B=\kappa^{3/2}\int dp\,dp'\,dq\,dq'\,a^*(q)a^*(q')a(p)a(p')\mathcal{V}_B(q,q',p,p')\,e^{-\kappa(p+p')^2-\kappa(q+q')^2} \qquad (1.9)$$

with $\mathcal{V}_B(q,q',p,p')=-\mathcal{V}_B(q',q,p,p')$ etc., in order to respect the Fermi-nature of a's. This potential has the property

$$\begin{aligned}\|V\|&<\infty && \text{for }\kappa<\infty\\ \|V\|&\to\infty && \text{for }\kappa\to\infty\end{aligned}$$

Despite this divergence, potential (1.9) may still generate a well-defined time evolution. The strong resolvent convergence in (1.8) is essential, weak convergence would not be enough since it does not guarantee the automorphism property

$$\tau_\kappa^t(ab)=\tau_\kappa^t(a)\tau_\kappa^t(b)\ \to\ \tau_\infty^t(ab)=\tau_\infty^t(a)\tau_\infty^t(b)\,.$$

Note that the parameter κ plays in this construction the role of the volume from the considerations in [2].

In the mean-field regime we want an effective Hamiltonian

$$H_B''=\int dp\,[\omega(p)a^*(p)a(p)+\Delta_M(p)a^*(p)a(p)]\,. \qquad (1.10)$$

Here the KMS-state is defined for the operators a,a^* themselves and one should rather smear by means of

$$e^{-\kappa(q-p)^2-\kappa(q'-p')^2}v(p)v(p') \qquad (1.11)$$

instead of (1.7), thus concluding that

$$\text{s-}\lim_{\kappa\to\infty}\int dp\,dq\,e^{-\kappa(q-p)^2}a^*(q)a(p)\mathcal{V}_M(q,q',p,p')=-\int dp\,\frac{\mathcal{V}_M(p,q',p,p')}{1+e^{\beta(\varepsilon(p)-\mu)}}\,, \qquad (1.12)$$

with $\varepsilon(p)=\omega(p)+\Delta_M(p)$. Relation (1.12) then suggests another starting potential

$$V_M=\kappa^{3/2}\int dp\,dp'\,dq\,dq'\,a^*(q)a^*(q')a(p)a(p')\mathcal{V}_M(q,q',p,p')\,e^{-\kappa(q-p)^2-\kappa(q'-p')^2} \qquad (1.13)$$

with the same symmetry for the density $\mathcal{V}_M$ as in (1.9). However, in both cases a Gaussian form factor in the smearing functions (1.7),(1.11) has been chosen just for simplicity. In principle, this might be C_o^∞ functions which have the δ-function as a limit.

2 The model

Consider the following Hamiltonian

$$H = H_{kin} + V_B + V_M \,, \tag{2.1}$$

where H_{kin} is the kinetic term and V_B, V_M are given by (1.9),(1.13). The solvability of the model for $\kappa \to \infty$ depends on whether or not it would be possible to replace (2.1) by an equivalent Hamiltonian that might be readily diagonalized. The object of interest is the commutator of, say, a creation operator with the potential. With (1.8), (1.12) taken into account, it reads

$$[a(k), V] = 2 \int dp \left\{ c(p)s(p) [p] \, \mathcal{V}_B(k, -k, p, -p) a^*(-k) + \mathcal{V}_M(p, k, p, k) \, \{p\} \, a(k) \right\} \tag{2.2}$$

The Bogoliubov-type Hamiltonian for our problem should be a combination of (1.1) and (1.10), that is of the form

$$H_B = \int dp \left\{ a^*(p)a(p)[\omega(p) + \Delta_M(p)] + \frac{1}{2}\Delta_B(p)[a^*(p)a^*(-p) + a(-p)a(p)] \right\} \tag{2.3}$$

This Hamiltonian becomes equivalent to the model Hamiltonian (2.1), provided the commutator $[a(k), H_B - H_{kin}]$ equals (2.2). Thus we are led to a system of two coupled "gap equations"

$$\frac{1}{2}\Delta_M(k) = \int \mathcal{V}_M(k, p) \left\{ \frac{c^2(p)}{1 + e^{\beta(\overline{W}(p) - \mu)}} + \frac{s^2(p)}{1 + e^{-\beta(\overline{W}(p) - \mu)}} \right\} dp \tag{2.4}$$

$$\Delta_B(k) = \int \mathcal{V}_B(k, p) \frac{\Delta_B(p)}{\overline{W}(p)} \tanh \frac{\beta(\overline{W}(p) - \mu)}{2} dp \,, \tag{2.5}$$

with

$$\overline{W}(p) = \sqrt{[\omega(p) + \Delta_M(p)]^2 + \Delta_B^2(p)} \,. \tag{2.6}$$

c (and thus s, Eq.(1.2)) are determined by either of the following conditions

$$c^2(p) - s^2(p) = [\omega(p) + \Delta_M(p)]/\overline{W}(p) \,, \qquad 2c(p)s(p) = \Delta_B(p)/\overline{W}(p) \,. \tag{2.7}$$

The temperature and the interaction-strenght dependence of the system (2.4–7) encode the solvability of the model [6].

3 High T_c case

We are now looking for a mechanism for high temperature superconductivity, i.e. a high T_c where Δ_B starts to vanish. If we make the ansatz

$$\mathcal{V}_B(k, p) = \lambda_B v(k)v(p) \,, \qquad \int v^2(p)dp = 1 \,, \qquad v(p) = -v(-p) \,,$$

then (2.5)becomes

$$\Delta_B(k) = \lambda_B v(k) \int dp \frac{v(p)\Delta_B(p)}{\overline{W}(p)} \tanh \frac{\beta(\overline{W}(p) - \mu)}{2} \, .$$

For $\lambda_B < 0$ we must have $\overline{W} < \mu$ and since $\tanh x < x \, , \forall x > 0$, we conclude that

$$T < \frac{|\lambda_B|}{2} \int dp v^2(p) \left(\frac{\mu}{\overline{W}(p)} - 1 \right) \, .$$

If Δ_B starts to vanish, $\overline{W}(p) = |\omega(p) + \Delta_M(p)|$, so if $\Delta_M < 0$ and near $\omega(p)$, T_c can become arbitrarily high

$$T_c < \frac{|\lambda_B|}{2} \left(-1 + \mu \int \frac{dp v^2(p)}{|\omega(p) + \Delta_M(p)|} \right) \, .$$

Thus a negative mean field which almost cancels the kinetic energy ω gives the electrons so much mobility to respond to $\lambda_B < 0$ that even at high temperatures a gap Δ_B can develope. There is a small problem since $\Delta_B(-k) = -\Delta_B(k)$. However $v(k)$ need not be continuous and since only Δ_B^2 enters in $\overline{W}$ the gap parameter $\Delta_B^2(0)$ can effectively be $\neq 0$. This problem disappears if we include spin and thus have $a_\uparrow(p)a_\downarrow(-p)$ in V_B.

4   Conclusion

Our model has four parameters, $\lambda_M, \lambda_B, \mu, T$, but by scaling only their ratios are essential. For infinite temperature $\beta = 0$ Eqs.(3.1–3) admit only the mean field solution $\Delta_B = 0 \, , \Delta_M = \lambda_M, \, \overline{W} = \mu + \lambda_M$. By lowering the temperature one meets also the BCS-type solution but in a rather complicated region in the 3–dimensional parameter space.

Whenever λ_B is positive, it must be also $> \mu$. Also for negative λ_B, λ_M and $\lambda_M > -\mu$ there exists a finite gap for λ_B. A perturbation theory with respect to λ_B is in general doomed to failure since for no point on the $\lambda_B = 0$ axis there is a neighbourhood full of the $\Delta_B \neq 0$ phase.

It is interesting that without a mean field (the $\lambda_M = 0$ axis) there are superconducting solutions only for $\lambda_B > \mu$. An attractive mean field ($\lambda_M < 0$) stimulates superconductivity since then it also appears for negative λ_B. However, too strong mean field attraction destroyes it again.

The most remarkable fact is that whilst for $\lambda > 0$ the temperature for a superconducting phase is limited as in the BCS theory by $T \ll (\lambda_B - \mu)/2$, in the new phases for $\lambda_B < 0$, $\lambda_M < 0$ we only get $T < |\lambda_B||\lambda_M|/2(\mu - |\lambda_M|)$ and thus for $\lambda_M \to -\mu$, T can become arbitrarily big.

Acknowledgements

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